Instructions and Sample Problems for Using the MACCS/HYSPLIT Capability

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Introduction

The capability to use HYSPLIT atmospheric transport and dispersion results has been integrated with MACCS and serves as an alternative to the original Gaussian plume segment model. The process of using this model starts with downloading meteorological files from the Air Resources Laboratory, which is under the National Oceanographic and Atmospheric Administration, (NOAA). These files are processed by the HYSPLIT modeling software, available from NOAA, optionally using a batch process and python scripts designed for this MACCS application. The output files from running the HYSPLIT application can then be linked to WinMACCS, a graphical interface to MACCS. Additionally, the MacMetGen application is available to create a MACCS formatted meteorological file from the files downloaded from NOAA or other source of meteorological data.

HyGridConvert can be run independently of WinMACCS to create air and ground concentration files that are compatible with MACCS. The MACCS-formatted files can be linked to the WinMACCS project or used directly by MACCS.

The explanations and examples following this file are based on WinMACCS 3.11.6 and the MACCS-HYSPLIT tools suite. These codes and tools are available from Sandia National Laboratories.

Installing HYSPLIT and Other Software

Python

Install Python version 3.3 or later. This is a command language interpreter that is used to generate HYSPLIT files using a Sandia-provided Python3 script, GenHysplit. Python downloads can be found at the following site:

https://www.python.org/downloads/

The process described in this document was tested using Python 3.7.

Linux:

The following can be added to a bash script or can be run from the command line:

```
# Make sure proxy is set up when using a proxy, e.g., export HTTPS_PROXY=http://wwwproxy.sandia.gov:80 export HTTP_PROXY=${HTTPS_PROXY} export http_proxy=${HTTPS_PROXY} export https_proxy=${HTTPS_PROXY}
```

Important Note: Versions >= 3.7 must have libffi installed on system for ctypes

```
curl http://mirror.centos.org/centos/6/os/x86_64/Packages/libffi-devel-3.0.5-3.2.el6.x86_64.rpm > libffi-devel-3.0.5-3.2.el6.x86_64.rpm sudo rpm -ivv libffi-devel-3.0.5-3.2.el6.x86_64.rpm rm libffi-devel-3.0.5-3.2.el6.x86_64.rpm
```

Change as needed

```
PYTHON_VERSION=3.7.0
PYTHON_SHORT_VERSION=3.7
```

Change dir when needed (This is an example location)

```
PYTHON_INSTALL_DIR=/projects/python${PYTHON_SHORT_VERSION}
```

Make directory for new python

```
rm -rf ${PYTHON_INSTALL_DIR}
mkdir ${PYTHON_INSTALL_DIR}
```

Important Note: Versions >= 3.7 need to make sure newer openssl installed

```
OPENSSL VERSION=1.1.0h
```

Download OpenSSL and install to Python dir

```
curl -k https://www.openssl.org/source/openssl-${OPENSSL VERSION}.tar.gz > openssl-
   ${OPENSSL VERSION}.tar.gz
   tar xvf openssl-${OPENSSL VERSION}.tar.gz
   rm openssl-${OPENSSL VERSION}.tar.gz
   mkdir -p ${PYTHON_INSTALL_DIR}/openssl/usr/local/ssl
   mv openssl-${OPENSSL VERSION} ${PYTHON INSTALL DIR}/
   cd ${PYTHON INSTALL DIR}/openssl-${OPENSSL VERSION}
   ./config --prefix=${PYTHON INSTALL DIR}/openssl --
   openssldir=${PYTHON_INSTALL_DIR}/openssl/usr/local/ssl
   make install
   cd -
   rm -rf ${PYTHON INSTALL DIR}/openssl-${OPENSSL VERSION}
# Download Python
   curl -k https://www.python.org/ftp/python/${PYTHON_VERSION}/Python-${PYTHON_VERSION}.tgz
   > Python-${PYTHON VERSION}.tgz
# Extract and remove tgz
   tar -xvf Python-${PYTHON VERSION}.tgz
   rm Python-${PYTHON_VERSION}.tgz
# Change dir to download Python
   cd Python-${PYTHON VERSION}
   ./configure --prefix=${PYTHON INSTALL DIR} --with-openssl=${PYTHON INSTALL DIR}/openssl
   make install
# Remove Python download
   cd ..
   rm -rf Python-${PYTHON_VERSION}
# Install site-packages
   cd ${PYTHON INSTALL DIR}/bin
# Ensure pip, setuptools, and wheel up-to-date
   ./python${PYTHON_SHORT_VERSION} -m pip install --upgrade pip setuptools wheel
   # Install specific packages
   SITE_PACKAGES=(numpy mpi4py)
   for i in ${SITE PACKAGES[@]}; do
     ./python${PYTHON_SHORT_VERSION} -m pip install ${i}
   done
   cp f2py f2py${PYTHON SHORT VERSION}
```

How to run installed python (Up to user to add alias to bashrc or add

```
#${PYTHON_INSTALL_DIR}/bin to path)
${PYTHON_INSTALL_DIR}/bin/python3.7
```

Windows:

After installing Python, add the following windows paths to the Environment Variables.

Example paths:

```
C:\Users\kImcfad\AppData\Local\Programs\Python\Python37; C:\Users\kImcfad\AppData\Local\Programs\Python\Python37\Scripts
```

To do this, open the Control Panel. Open the System Properties window, Advanced tab, and click on the Environment Variables button.

Add the python installation folder and the Scripts sub folder to the system PATH environment variable.

Numpy, a python scientific computing package, is required. Not all versions of python come packaged with numpy. The installation of numpy can be tested by starting python either from a command window or the IDLE application and typing the following command:

```
>>> import numpy
```

If numpy is properly linked to python, there will be no error message displayed.

If numpy was not installed, it needs to be installed by using a python package manager such as pip. Open a command window, and type the following command:

```
>pip install numpy
```

If your organization has a proxy server, this may need to be specified also as shown in the following example:

```
>pip install –proxy server.org.name:PP numpy
```

where server.org.name is the proxy server, and PP is the prescribed port number. This information is available through your organizations computer support personal.

MPI

Install MPI (message passage interface) for Python (MPI4PY). This allows GenHysplit to access multiple processors through calls to the MPI interface, allowing the meterological files to be processed faster than using a single processor. Even if only one processor is used, MPI must still be installed.

Linux:

Install Openmpi version 1.8 or later, which can be found at the following site:

```
https://www.open-mpi.org/software/ompi/v3.1/
```

Make sure proxy is set up when using a proxy, for example

```
export HTTPS_PROXY=http://wwwproxy.sandia.gov:80
export HTTP_PROXY=${HTTPS_PROXY}
export http_proxy=${HTTPS_PROXY}
export https_proxy=${HTTPS_PROXY}
```

Download and install openmpi

```
curl -k <a href="https://download.open-mpi.org/release/open-mpi/v3.1/openmpi-3.1.2.tar.bz2">https://download.open-mpi.org/release/open-mpi/v3.1/openmpi-3.1.2.tar.bz2</a> > openmpi-3.1.2 tar.bz2 gunzip -c openmpi-3.1.2.tar.gz | tar xf - cd openmpi-3.1.2 ./configure --prefix=/usr/local <...lots of output...> make all install
```

Windows:

Download Microsoft MPI 8.1 and install both MPI (MSMpiSetup.exe) and the MPI software development kit (msmpisdk.msi). It is necessary to run both applications.

https://www.microsoft.com/en-us/download/details.aspx?id=55494

Version: 8.1.12438	Date Published: 6/16/2017
File Name:	File Size:
msmpisdk.msi	2.2 MB
MSMpiSetup.exe	5.2 MB

Add the path C:\Program Files\Microsoft MPI\bin to the system PATH environment variable

After this is done, link mpi with python with the following command:

```
>pip install mpi4py
```

HYSPLIT

Install HYSPLIT version 927 or later. HYSPLIT is a code managed by the Air Resources Laboratory, National Oceanic and Atmospheric Administration (NOAA). The user should register and obtain an account before downloading the files. A non-registered version may be

used but may not include all the updates available in the registered version. The registration form and instructions can be found at:

https://ready.arl.noaa.gov/HYSPLIT_register.php

Once registered, the ARL webmaster emails instructions for logging into the download page.

The source code or an executable is available for Linux. For Windows, download the registered (not public) version of Windows-based HYSPLIT. No source code is available for the Windows version.

HYSPLIT Sample Problem, Five Days of Data

Follow the instructions in the section Installing HYSPLIT and Other Software above to install software needed to complete this sample problem. The .ccd files generated in this sample problem are used in the section WinMACCS Sample Problem – HYSPLIT Fixed Start Time below.

Download Meteorological Files on Linux

- 1. Determine directory location for storage of meteorological files. Depending on the number of files, the required storage may be large. The files should be accessible from the location where GenHysplit is to be run. For the sample problem, the total size of the meteorological files is approximately 3GB.
- 2. Copy the get_weather_linux.sh and readme_linux.txt files into the meteorological file directory. These files can be found in the included distribution folder, GetWeather.
- 3. Open get_weather_linux.sh and modify for the sample problem settings as discussed in the readme_linux.txt file. For the sample problem, the modification results in downloading Global Data Assimilation System (GDAS) weather files that contain data on 0.5-degree latitude and longitude increments (0p5) for March 11-16, 2011.
 - a. Modify the value of MET to the desired file storage location
 - b. Modify the value of met_end to "_gdas0p5"
 - c. Modify the value of ftp_loc to "ftp://arlftp.arlhq.noaa.gov/archives/gdas0p5"
 - d. Modify the value of YY to "2011"
 - e. Modify the value of MM to "03"
 - f. Modify the value of DD to "11" "12" "13" "14" "15" "16"
- 4. Download needed data by typing the following command in the meteorological directory: >./get_weather_linux.sh

Download Meteorological Files on Windows

- 1. Determine directory location for storage of meteorological files. Depending on the number of files, the total file size may be large. The files should be accessible from where GenHysplit is to be run. For the test case the total size of the meteorological files is approximately 3 GB. Create this folder if it does not exit.
- 2. Copy the get_weather_windows.bat and readme_windows.txt files into the meteorological file directory. These files can be found in the distribution folder GetWeather.
- 3. Open get_weather_windows.bat in a text editor such as Notepad and modify for the sample problem settings as discussed in the readme_windows.txt file. This can be done either by right clicking on the .bat file and selecting edit, or starting the editor and opening the file. Do not double click on the .bat file because that causes the file to be executed. For the sample problem, the desired result is to download Global Data Assimilation System (GDAS) weather files that contain data on 0.5-degree latitude and longitude increments (0p5) for March 11-16, 2011. The new values indicated below

should not contain the quotes. For example, step d below asks to change the YY variable to "2011". The line should be entered as follows: set yy=2011. There should be no space between the variable and the equal sign or the equal sign and the value.

- a. Modify the value of MET to the desired file storage location. If the path has spaces, enclose the path with double quote marks.
- b. Modify the value of met_end to "_gdas0p5"
- c. Modify the value of ftp_loc to "ftp://arlftp.arlhq.noaa.gov/archives/gdas0p5/"
- d. Modify the value of YY to "2011"
- e. Modify the value of MM to "03"
- f. Modify the value of DD to "11 12 13 14 15 16"
- 4. The data can be downloaded by either double clicking the get_weather.bat file or by running the batch command directly in a command prompt window. This is done by opening the command application (cmd.exe), changing the folder to the location of the batch file, and then typing the command at the prompt as shown:
 - > get_weather_windows

Run MacMetGen

- 1. Determine the folder location for storage of the MacMetGen output files. The folder should be accessible from where you plan to run MacMetGen. MacMetGen is a windows executable. For the test case the total size of the MacMetGen output files is approximately 180 KB.
- 2. For the sample problem, copy the MacMetGen input file sample_MacMetGen.inp to a working folder and rename this file met_fs.inp. The example file is in the distribution folder \MacMetGen.
- 3. Open the met_fs.inp file in a text editor and modify for the sample problem settings. Detailed information about the format of this input file is described in the document MacMetGen 1.0.0 Users Guide.pdf, released with MacMetGen. The sample problem is intended to generate a MACCS-formatted weather file using GDAS0p5 weather data from March 11-16, 2011, for the Fukushima Daiichi NPP, for a 16-sector grid with 60-minute intervals using the dT/dZ stability class method. MACCS requires an input meteorological file with one years' worth of data. As less than one years' worth of meteorological data are provided, the output file will repeat the meteorological data until one years' worth is obtained to meet this requirement. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.
 - a. Do not modify line 7, retain the value 0 to create the surface data file.
 - b. Modify the path on line 9 to the path and name of the intermediary surface data file that MacMetGen will create.
 - c. Modify the latitude and longitude values on line 11 to "37.4230 141.0329".
 - d. Leave the value on line 13 as 1 indicating there is one set of meteorological files.

- e. Modify the first and last dates of interest on line 15 to "20110311 20110316".
- f. Modify the directory on line 17 to the location of the downloaded meteorological files.
- g. Leave the value on line 19 as blank, setting the weather file prefix to ".".
- h. Leave the value on line 21 as "_nam12", setting the weather file postfix to "gdas0p5".
- i. Modify the path on line 26 to the location of the MacMetGen output files with the specified name of the MACCS-formatted weather file.
- j. Leave the value on line 28 as 60, the number of minutes associated with each line in the output file.
- k. Modify the number of sectors on line 30 from 64 to 16.
- 1. Modify the value on line 32 to 0 setting the stability class to the algorithm dT/dz.
- m. Modify the morning mixing heights on line 34 to "300 300 300 300".
- n. Modify the afternoon mixing heights on line 36 to "1000 1000 1000 1000".
- 4. Navigate to the location of the MacMetGen executable in a command prompt. The command is then MacMetGen.exe -i "path\ met_fs.inp", where path indicates relative location to the input file as shown in the following example:
 - > MacMetGen -i input\ met_fs.inp"
- 5. MacMetGen should then run the sample problem. This can take several minutes. The file currently being processed is shown on the command prompt to help estimate progress.

Four files should be created in the specified output folder: 1) the output surface data file; 2) the MACCS-formatted weather file; 3) a *.stat file, which indicates the status of the run (should indicate "OK" after the run is complete); and 4) a *.log file, which contained a copy of the input file used and the output shown to the command prompt. The MACCS-formatted weather file can be compared with the "gdas0p5_dtdz.MET" file included in the Data folder of the project *Gaussian Fixed Start Time*.

Run GenHysplit

- 1. Determine the folder location for storage of the HYSPLIT output files. Depending on the number of files, the required storage may be large. The files should be accessible from where Python, OpenMPI (or Microsoft MPI), and HYSPLIT are installed, as well as the meteorological files. For the test case the total size of the HYSPLIT files is approximately 200 MB, but the total folder size with all intermediate results is 600 MB.
- 2. Place the GenHysplit.py, pyhysplit.py, and realization.py files in the folder where you are running GenHysplit. These files can be found in the distribution folder GenHysplit/source.
- 3. Place the GenHysplit input files where you want to store the input file. These files can be found in the distribution folder GenHysplit.

- 4. For the sample problem, rename sample_GenHysplit.inp to sample_problem_fs.inp. By default, when the input file is not specified on the instantiation line, GenHysplit expects the file to be named test.inp.
- 5. Open the sample_problem_fs.inp file in a text editor and modify for the sample problem settings. The sample problem models release each hour from March 11, 2011, to March 15, 2011, over a 12-hour period, for a range of 100 miles around the Fukushima Daiichi NPP with default HYSPLIT settings. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.
 - a. Modify the directory on line 9 to the location of the downloaded meteorological files.
 - b. Leave the default value on line 11 as blank.
 - c. Leave the default value on line 13 as 0.
 - d. Modify the directory on line 15 to the location of the HYSPLIT installation folder.
 - e. Modify the directory on line 17 to the location of the HYSPLIT output file.
 - f. Leave the default value on line 22 as 1.
 - g. Modify the values on line 24 to "20110311 20110315".
 - h. Modify the values on line 26 to "141 1 58 E".
 - i. Modify the values on line 28 to "37 25 16 N".
 - j. Leave the default value on line 30 as 0.
 - k. Leave the default value on line 32 as 10.
 - 1. The values on line 34 will not be used. Can be changed to anything.
 - m. Leave the default value on line 36 as 0.
 - n. Modify the value on line 38 to 12.
 - o. Leave the default value on line 40 as 15.
 - p. Leave the default value on line 42 as 1.
 - q. Modify the value on line 44 to 161.0.
 - r. Leave the default value on line 46 as 10.
 - s. Leave the default value on line 48 as 0.5.
 - t. Leave the default value on line 50 as 50.
 - u. Leave the default value on line 52 as 0.
 - v. Leave the default value on line 54 as 10.
 - w. Leave the default values on line 56 as "0.15332 0.28543 0.53138 0.98923 1.8416 3.4284 6.3825 11.882 22.120 41.179".
 - x. Leave the default values on line 58 as "1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0".
 - v. Leave the default values on line 60 as "0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0".
 - z. Leave the default value on line 62 as 2.
- 6. Execute GenHysplit.

Running on Linux

For running on a single processor, use the command:

mpirun -n 1 python3 <location of *.py files>GenHysplit.py -i <location and name of input file>

For submitting a job on to a Linux cluster with a SLURM queueing system with 60 processors, use the command:

salloc -n 60 mpirun python3 <location of *.py files>GenHysplit.pyt -i <location and name of input file>

Running on Windows

To view help and to verify that mpiexec has been correctly installed, type the command

>mpiexec

More help is available with the -help2 command. In this example, the output from the help command is piped into the more function. Tap the spacebar to get the next page of help.

>mpiexec -help2 | more

For running a single processor, the command is:

python.exe "completepath/GenHysplit.py" -i "completepath/sample_problem_fs.inp"

Where complete path indicates the location of the files needed as shown in the following example:

> python "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\GenHysplit.py" -i "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\sample_problem_fs.inp"

To take advantage of multiple cores that may be available, open Windows Task Manager to determine the number of cores available. On Windows 10, select the Performance tab. Notice the value of the variable "Cores" in this window. The number of cores is used for the value for n in the mpiexec command. For example, if the number of Cores is equal to 4, the mpiexec command would be as follows:

> mpiexec -n 4 python "completpath/GenHysplit.py" -i "completepath/sample_problem_fs.inp"

Once successfully finished, the completed set of HYSPLIT output files (.ccd files) is found in the specified directory (line 17 in input file) in the data directory. There should be 120 .ccd files, along with a copy of the input file used and a log file.

HYSPLIT Sample Problem, One Year of Data

Follow the instructions in the section Installing HYSPLIT and Other Software above to install software needed to complete this sample problem. The .ccd files generated in this sample problem are used in the section WinMACCS Sample Problem – HYSPLIT Weather Sampling below.

Download Meteorological Files on Linux

- 1. Determine directory location for storage of meteorological files. Depending on the number of files, the required storage may be large. The files should be accessible from the location where MacMetGen is to be run. For the sample problem, the total size of the meteorological files is approximately 152GB.
- 2. Copy the get_weather_linux.sh and readme_linux.txt files into the meteorological file directory. These files can be found in the included distribution folder, GetWeather.
- 3. Open get_weather_linux.sh and modify for the sample problem settings as discussed in the readme_linux.txt file. For the sample problem, the modification results in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for January 1 December 31, 2015.
 - a. Modify the value of MET to the desired file storage location
 - b. Modify the value of met_end to "_nam12"
 - c. Modify the value of ftp_loc to "ftp://arlftp.arlhq.noaa.gov/archives/nam12"
 - d. Modify the value of YY to "2015"
 - e. Modify the value of MM to "01" "02" "03" "04" "05" "06" "07" "08" "09" "10" "11" "12"
 - f. Modify the value of DD to "01" "02" "03" "04" "05" "06" "07" "08" "09" "10" "11" "12" "13" "14" "15" "16" "17" "18" "19" "20" "21" "22" "23" "24" "25" "26" "27" "28" "29" "30" "31"
- 4. Download needed data by typing the following command in the meteorological directory: >./get_weather_linux.sh
- 5. Additional meteorological data are needed for the HYSPLIT file generation. These additional files cover the periods before January 1, 2015 and after December 31, 2015 that are used in HYSPLIT calculations below. They are not needed to generate the MACCS formatted meteorological file.
 - a. For the period before January 1, 2015, open the get_weather_linux.sh file and modify the settings as discussed in the readme_linux.txt file and above. For this period, the modification should be made to result in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for December 29 31, 2014. Then execute the script as discussed above.
 - b. For the period after December 31, 2015, open the get_weather_linux.sh file and modify the settings as discussed in the readme_linux.txt file and above. For this period, the modification should be made to result in downloading North American

Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for January 1 – February 10, 2016. Then execute the script as discussed above.

Download Meteorological Files on Windows

- 1. Determine directory location for storage of meteorological files. Depending on the number of files, the total file size may be large. The files should be accessible from where MacMetGen is to be run. For the test case the total size of the meteorological files is approximately 152 GB. Create this folder if it does not exit.
- 2. Copy the get_weather_windows.bat and readme_windows.txt files into the meteorological file directory. These files can be found in the distribution folder GetWeather.
- 3. Open get_weather_windows.bat in a text editor such as Notepad and modify for the sample problem settings as discussed in the readme_windows.txt file. This can be done either by right clicking on the .bat file and selecting edit, or starting the editor and opening the file. Do not double click on the .bat file because that causes the file to be executed. For the sample problem, the desired result is to download North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for January 1 December 31, 2015. The new values indicated below should not contain the quotes. For example, step d below asks to change the YY variable to "2015". The line should be entered as follows: set yy=2015. There should be no space between the variable and the equal sign or the equal sign and the value.
 - a. Modify the value of MET to the desired file storage location. If the path has spaces, enclose the path with double quote marks.
 - b. Modify the value of met_end to "_nam12"
 - c. Modify the value of ftp_loc to "ftp://arlftp.arlhq.noaa.gov/archives/nam12/"
 - d. Modify the value of YY to "2015"
 - e. Modify the value of MM to "01 02 03 04 05 06 07 08 09 10 11 12"
 - f. Modify the value of DD to "01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31"
- 4. The data can be downloaded by either double clicking the get_weather.bat file or by running the batch command directly in a command prompt window. This is done by opening the command application (cmd.exe), changing the folder to the location of the batch file, and then typing the command at the prompt as shown:

 > get_weather_windows
- 5. Additional meteorological data is needed for the HYSPLIT file generation. These additional files cover the periods before January 1, 2015 and after December 31, 2015 that are used in HYSPLIT calculations below. They are not needed to generate the MACCS formatted meteorological file.
 - a. For the period before January 1, 2015, open the get_weather_windows.bat in a text editor such as Notepad and modify the settings as discussed in the readme_windows.txt file and above. For this period, the modification should be

- made to result in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for December 29 31, 2014. Then execute the script as discussed above.
- b. For the period after December 31, 2015, open the get_weather_windows.bat in a text editor such as Notepad and modify the settings as discussed in the readme_windows.txt file and above. For this period, the modification should be made to result in downloading North American Mesoscale (NAM) weather files that contain data on 12-km by 12-km (12) for January 1 February 10, 2016. Then execute the script as discussed above.

Run MacMetGen

- 1. Determine the folder location for storage of the MacMetGen output files. The folder should be accessible from where you plan to run MacMetGen. MacMetGen is a windows executable. For the test case the total size of the MacMetGen output files is approximately 644 KB.
- 2. For the sample problem, copy the MacMetGen input file sample_MacMetGen.inp to a working folder and rename this file met_ws.inp. The example file is in the distribution folder \MacMetGen.
- 3. Open the met_ws.inp file in a text editor and modify for the sample problem settings. Detailed information about the format of this input file is described in the document MacMetGen 1.0.0 Users Guide.pdf, released with MacMetGen. The sample problem is intended to generate a MACCS-formatted weather file using NAM12 weather data from 2015, for a fictitious site located at latitude 36.19306, longitude -115.65463, for a 16-sector grid with 60-minute intervals using the dT/dZ stability class method. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.
 - a. Do not modify line 7, retain the value 0 to create the surface data file.
 - b. Modify the path on line 9 to the path and name of the intermediary surface data file that MacMetGen will create.
 - c. Modify the latitude and longitude values on line 11 to "36.19306 -115.65463".
 - d. Leave the value on line 13 as 1 indicating there is one set of meteorological files.
 - e. Modify the first and last dates of interest on line 15 to "20150101 20151231".
 - f. Modify the directory on line 17 to the location of the downloaded meteorological files.
 - g. Leave the value on line 19 as blank, setting the weather file prefix to "".
 - h. Leave the value on line 21 as "_nam12", setting the weather file postfix to " nam12".
 - i. Modify the path on line 26 to the location of the MacMetGen output files with the specified name of the MACCS-formatted weather file.

- j. Leave the value on line 28 as 60, the number of minutes associated with each line in the output file.
- k. Modify the number of sectors on line 30 from 64 to 16.
- 1. Modify the value on line 32 to 0 setting the stability class to the algorithm dT/dz.
- m. Modify the morning mixing heights on line 34 to "300 300 300 300".
- n. Modify the afternoon mixing heights on line 36 to "1000 1000 1000 1000".
- 4. Navigate to the location of the MacMetGen executable in a command prompt. The command is then MacMetGen.exe -i "path\ met_ws.inp", where path indicates relative location to the input file as shown in the following example:
 - > MacMetGen -i input\ met_ws.inp"
- 5. MacMetGen should then run the sample problem. This can take between one and several hours. The file currently being processed is shown on the command prompt to help estimate progress.
- 6. Four files should be created in the specified output folder: 1) the output surface data file; 2) the MACCS-formatted weather file; 3) a *.stat file, which indicates the status of the run (should indicate "OK" after the run is complete); and 4) a *.log file, which contained a copy of the input file used and the output shown to the command prompt. The MACCS-formatted weather file can be compared with the "FicticiousSite_dtdz.MET" file included in the Data folder of the project *Gaussian Weather Sampling*.

Run GenHysplit

Follow the instructions in the "Installing HYSPLIT and other software" section above to install software needed to complete this part of the sample problem. The .ccd files generated in this sample problem can be used in the "WinMACCS sample problem – HYSPLIT weather sampling" section below.

- 1. Determine the folder location for storage of the HYSPLIT output files. Depending on the number of files, the required storage may be large. The files should be accessible from where Python, OpenMPI (or Microsoft MPI), and HYSPLIT are installed, as well as the meteorological files. For the test case the total size of the HYSPLIT files is approximately 100 GB, but the total folder size with all intermediate results is 300 GB.
- 2. Place the GenHysplit.py, pyhysplit.py, and realization.py files in the folder where you are running GenHysplit. These files can be found in the distribution folder GenHysplit/source.
- 3. Place the GenHysplit input files where you want to store the input file. These files can be found in the distribution folder GenHysplit.
- 4. For the sample problem, rename sample_GenHysplit.inp to sample_problem_ws.inp. By default, when the input file is not specified on the instantiation line, GenHysplit expects the file to be named test.inp.
- 5. Open the sample_problem_ws.inp file in a text editor and modify for the sample problem settings. The sample problem models release each hour from December 29, 2014 to

February 9, 2016, over a 12-hour period, for a range of 100 miles around a fictitious site, for three release heights with default HYSPLIT settings. Do not add any additional comment lines. The number of comments and their positions in the file are fixed. However, comment lines can be modified. Do not enclose any paths with quotes. Spaces in path names are supported. Parameters on lines are in free format, separated by spaces.

- a. Modify the directory on line 9 to the location of the downloaded meteorological files.
- b. Leave the default value on line 11 as blank.
- c. Leave the default value on line 13 as 0.
- d. Modify the directory on line 15 to the location of the HYSPLIT installation folder.
- e. Modify the directory on line 17 to the location of the HYSPLIT output file.
- f. Leave the default value on line 22 as 1.
- g. Modify the values on line 24 to "20141229 20160209".
- h. Modify the values on line 26 to "115 58 55 W".
- i. Modify the values on line 28 to "36 11 35 N".
- j. Leave the default value on line 30 as 0.
- k. Modify the value on line 32 to "10 50 100".
- 1. The values on line 34 will not be used. Can be changed to anything.
- m. Leave the default value on line 36 as 0.
- n. Modify the value on line 38 to 12.
- o. Leave the default value on line 40 as 15.
- p. Leave the default value on line 42 as 1.
- q. Modify the value on line 44 to 161.0.
- r. Leave the default value on line 46 as 10.
- s. Leave the default value on line 48 as 1.0.
- t. Leave the default value on line 50 as 50.
- u. Leave the default value on line 52 as 0.
- v. Leave the default value on line 54 as 10.
- w. Leave the default values on line 56 as "0.15332 0.28543 0.53138 0.98923 1.8416 3.4284 6.3825 11.882 22.120 41.179".
- x. Leave the default values on line 58 as "1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0".
- y. Leave the default values on line 60 as "0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0".
- z. Leave the default value on line 62 as 2.
- 6. Execute GenHysplit.

Running on Linux

For running on a single processor, use the command:

mpirun -n 1 python3 <location of *.py files>GenHysplit.py -i <location and name of input file>

For submitting a job on to a Linux cluster with a SLURM queueing system with 60 processors, use the command:

salloc -n 60 mpirun python3 <location of *.py files>GenHysplit.pyt -i <location and name of input file>

Running on Windows

To view help and to verify that mpiexec has been correctly installed, type the command

>mpiexec

More help is available with the -help2 command. In this example, the output from the help command is piped into the more function. Tap the spacebar to get the next page of help.

```
>mpiexec -help2|more
```

For running a single processor, the command is:

```
python.exe "completepath/GenHysplit.py" -i "completepath/sample_problem_ws.inp"
```

Where complete path indicates the location of the files needed as shown in the following example:

> python "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\GenHysplit.py" -i "D:\Software Development\WinMACCS\Deploy WinMACCS 3.11.3 with HYSPLIT\Generate HYSPLIT Files\sample problem ws.inp"

To take advantage of multiple cores that may be available, open Windows Task Manager to determine the number of cores available. On Windows 10, select the Performance tab. Notice the value of the variable "Cores" in this window. The number of cores is used for the value for n in the mpiexec command. For example, if the number of Cores is equal to 4, the mpiexec command would be as follows:

```
> mpiexec -n 4 python "completpath/GenHysplit.py" -i "completepath/sample_problem_ws.inp"
```

Once successfully finished, the completed set of HYSPLIT output files (.ccd files) is found in the specified directory (line 17 in input file) in the data directory. There should be 29,376 .ccd files, along with a copy of the input file used and a log file.

Using the HYSPLIT Model from WinMACCS

Overview

HYSPLIT is executed independently of WinMACCS. Running HYSPLIT to process a year of weather data is a CPU-intensive process that requires multiple processors to run over a reasonable time (several days). This process must use data consistent with the WinMACCS model settings for the particle bin sizes and the latitude and longitude of the site. The number of particle size bins to be used in WinMACCS, variable NPSGRP, should be equal to the HYSPLIT input for the number of particle size bins and their sizes should be set consistently. The latitude and longitude defined in WinMACCS, variables Latitude and Longitude, should agree with the values in the HYSPLIT input files. If any of these values are changed in the WinMACCS model, HYSPLIT needs to be run again with the new values. The output files from HYSPLIT are named according to the date and the time modeled. The file extension of the HYSPLIT output files is mcd. For example, 2007122913H001.mcd contains data corresponding to a release that occurs during hour 13 (from 12:00 to 13:00) on 12/29/2007. H001 indicates that the data are for a release height of 10 m.

Create MACCS-HYSPLIT Files

The output from HYSPLIT is organized in a uniform rectangular or polar grid. HyGridConvert, a utility that is bundled with WinMACCS, can convert HYSPLIT data from either a uniform rectangular or polar coordinate system to the polar coordinated system used by MACCS. The coordinate system is characterized by the variables SPAEND (defines the outer radii of each ring) and NUMCOR (defines the number of sectors). HyGridConvert is a software tool developed at Sandia and is run from the WinMACCS interface to convert output from the HYSPLIT data files to data files compatible with MACCS. This tool can also be run independently without using the WinMACCS interface.

Before running HyGridConvert, the following variables need to be defined in the WinMACCS interface:

- Latitude
- Longitude
- NUMCOR
- SPAEND

HyGridConvert can be rerun if new values are chosen for NUMCOR and SPAEND; HYSPLIT must be rerun if the latitude or longitude of the release location change.

The *Convert HYSPLIT files to MACCS Grid* form is opened by selecting the main menu item *PreProcessing/Create MACCS-HYSPLIT files*. The *Convert HYSPLIT files to MACCS Grid* form opens as shown in Figure 1.

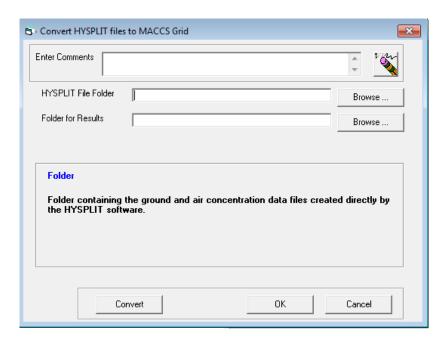


Figure 1. Convert HYSPLIT files to MACCS Grid Form

The inputs on this form are folder names that are defined by clicking on the *Browse*... buttons. If either of these folders are on the network, the paths need to be mapped to drive letters in Windows for this process to work correctly. In other words, if the path of the folder starts with two back or forward slashes, the drive needs to be mapped using Windows Explorer, so it can be reference as a letter followed by a colon (e.g., X:\my local drive\HYSPLIT output).

The variable *HYSPLIT File Folder* is the folder containing the HYSPLIT result files. These files can be identified by the .ccd extension. All files with the extension .ccd are processed in the folder specified when the *Convert* button is clicked. A set of .ccd files representing a year of data typically occupy about 40 GB of storage.

The variable *Folder for Results* is the folder for the HyGridConvert output. It is acceptable to have existing files in this folder. However, when files are created by HyGridConvert with the same name as the existing files, the old files are overwritten. The files output from HyGridConvert are referred to as MACCS-HYSPLIT atmospheric files and have the extension .mcd.

When HyGridConvert is run, a status folder is created in the same folder as the MACCS-HYSPLIT files. This folder is identified by the time of the run, for example Status_08_21_2018_18_46_13 corresponds to a HyGridConvert run that was run on August 21, 2018 at time 18:46:13. This folder contains the HyGridConvert input file, HyGridConvert_site.inp, a status file, status.stat, and a detailed output file, status.log. The input file is created by WinMACCS. The status file contains either the character string OK if the execution was error free, or an error message from HyGridConvert if there was an error detected. Calculation details are saved in status.log.

To aid the user in organizing the MACCS-HYSPLIT files, the concept of a Data Repository was implemented. Because the files typically can take up 2 GB of data for a single year, this feature conserves space by allowing the same set of files to be used by different WinMACCS projects. The Data Repository is a folder that can be specified in the WinMACCS.ini file found in the Program Files (x86)/WinMACCS folder as shown in the following example:

REPOSITORY_DIR "D:\WinMACCS Projects\Repository"

If this parameter is not defined, it is assumed that the repository is in the following folder located in the user's documents folder:

"\WinMACCS Projects\Repository\"

HyGridConvert is run when the *Convert* button is clicked. A command window displays the names of the files as they are processed. The status of the run is shown in the WinMACCS Results window. For each release height, there are 8760 files generated by this process for a 365-day year; 8784 are generated for a 366-day year. After HyGridConvert finishes processing, the following line is printed in the WinMACCS Results window:

HyGridConvert execution SUCCESSFUL.

Define WinMACCS Parameters

The following steps lead to a WinMACCS project that uses HYSPLIT files to model the atmospheric transport in MACCS.

Select the HYSPLIT model

The HYSPLIT transport model and the weather sampling method are selected by opening the Project Properties form shown in Figure 2.

- The model is chosen on the *Scope* tab. Select the radio button labeled *HYSPLIT*. Notice that the dispersion model and plume meander model selections are not available on the *Transport* tab when the HYSPLIT model is selected.
- Clicking on the Weather tab, it can be observed that *Constant Weather* (METCOD=4) and *User Supplies 120 Weather Points* (METCOD=3) are not available. Choosing *Fixed Start Time* means that exactly one weather sequence is executed. The other sampling methods corresponding to METCOD=2 and 5 involve multiple, sampled, weather sequences. *Adjust Mixing Height Based on Time of Day* is not available with the HYSPLIT option.

Clicking *OK* saves the changes.

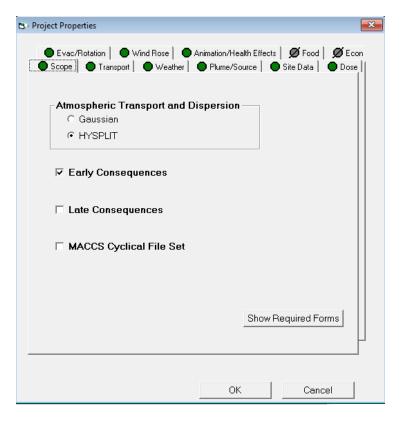


Figure 2. Selecting the HYSPLIT model

Specify a metrological file

The Fixed Start Time model in conjunction with the HYSPLIT transport model does not require a meteorological file. However, the weather bin sampling methods (METCOD=2) do require a 365-day meteorological file. The HYSPLIT model within MACCS supports 15-, 30-, and 60-minute time intervals in the standard (365-day) MACCS meteorological data file. A specific file is selected by opening the *GENERAL/File Specifications/Meteorological File* form and selecting the meteorological file. Clicking OK saves the changes. HYSPLIT data files are in UTC (Greenwich Mean Time). The standard meteorological data file is generally based on a time zone local to the site. This potential difference in time frames between the two files is an inconsistency that can result in an incorrect assignment of weather bins. This can be fixed by modifying the standard meteorological file to be consistent with UTC. This inconsistency can be avoided if the meteorological data file is created using the same weather files used when running HYSPLIT. A software product, MacMetGen, is available to create these files.

Specify location of the MACCS-HYSPLIT files

Specifying the location of the MACCS-HYSPLIT atmospheric transport files is done by opening the *GENERAL/File Specifications/HYSPLIT Converted Folder* form and defining the location of the MACCS-HYSPLIT files. Unlike other files selected in WinMACCS, such as the site data file, the files are not copied to the project Data folder. Instead, a repository folder is specified

that contains the atmospheric transport files. This allows different projects to use the same HYSPLIT data and reduces the storage requirements.

MACCS-HYSPLIT files is the path where the MACCS-HYSPLIT files reside.

Variable Name	Definable	Туре	Dimensions	Allowed Values
MACCS- HYSPLIT files	Yes	Folder	None	Legal path on computer, including mapped drives but excluding network drives

Specify the site location

Specifying the site location is done by opening the *ATMOS/Weather/Site Location* form. These values are compared with the latitude and longitude written to the MACCS-HYSPLIT files when the user clicks the *Run Simulation* button and before the MACCS simulation is initiated. The two sets of latitude and longitude values must match.

Define the forms in the HYSPLIT Transport Parameters category *File extensions and lower bounds*

HYSPLIT input parameters specify either the release height or the power level associated with the created dataset. For MACCS to correctly identify the files to use, each set of MACCS-HYSPLIT data files must be identified. This is done by specifying the postfix portion of the file name (ex: H001 is the postfix portion of file 2008010100H001.mcd).

Variable HY_NUMPRE is the number of MACCS-HYSPLIT data file sets.

Variable HY_PREFIX is a vector of length HY_NUMPRE. The values determine the expected names of the MACCS-HYSPLIT files. The character string is either in the format Hxxx or Pxxx, where xxx corresponds to three digits. Hxxx represents a release height of xxx*10m. Pxxx represents a power level of xxx*0.1MW. For example, H001 corresponds to 10 meters, P050 corresponds to 5 MW.

When multiple sets of release heights or power levels are used, the variable HY_LOWER is used to determine when to transition from one set to another. Variable HY_LOWER is the lower bound of either the height or the power corresponding to HY_PREFIX. For example, for a set of release heights of H001, H005 and H020 (release heights of 10, 50 and 200 meters) the HY_LOWER values of 0, 30, and 100 meters indicate that the H001 file set is to be used for

releases between 0 and 30 meters, the H005 file set for releases between 30 and 100 meters, and the H020 file set for releases above 100 meters.

Variable Name	Definable	Type	Dimensions	Allowed Values
HY_NUMPRE	Yes	Integer	None	1 to 10
HY_PREFIX	Yes	String of length 4	HY_NUMPRE	Prefix of MACCS- HYSPLIT data files. The first character must be H (for height) or P (for power).
HY_LOWER	Yes	Real	HY_NUMPRE	[0, 1.0E5]

Fixed start time data

If *Fixed Start Time* is selected on the *Project Properties* form, then only a single weather sequence is run. For either fixed start time or weather sampling, the starting date and time for each weather trial are associated with the plume denoted by MAXRIS, the plume of maximum risk, defined on the *Release Description/Plume of Maximum Risk* form.

The variables on the ATMOS/HYSPLIT Transport/Fixed Start Time Data form are as follows:

HY_FIXED identifies the date when the weather sequence begins in UTC. This is entered in MM/DD/YYYY format. For example, "01/31/2008" is a valid string.

HY_HOUR identifies the starting hour of the weather trial based on 24 hours in a day in UTC. Hour 1 begins at midnight, hour 2 begins at 1:00 AM, etc.

Information required for the Gaussian and HYSPLIT models when running a fixed-start-time case are similar, but they are specified on two separate forms. An important distinction is that the Gaussian model requires a Julian day and hour; whereas, the HYSPLIT model requires a date and hour. For the purpose of comparing the two models, the user needs to choose these separate inputs so that they match, accounting for the difference in time zones. For example, the variables ISTRDY and ISTRHR may need to be adjusted to correspond to UTC time when comparing results between the models (e.g., subtracting the difference between the US time zone and Greenwich Mean Time).

Variable Name	Definable	Туре	Dimensions	Allowed Values
HY_FIXED	Yes	String	None	10-character string of format MM/DD/YYYY
HY_HOUR	Yes	Integer	None	1 to 24

Weather sampling

When multiple weather sequences are run (METCOD=2 or 5), with the start date determined by the chosen sampling algorithm, then a start and an end date are selected on the *ATMOS/HYSPLIT Transport/Transport Dates* form. For the current version of WinMACCS when using any of the weather sampling options, the start day must be January 1 of some year, and the end day must be December 31 of the same year for both 365- and 366-day years. However, this requirement is enforced only by MACCS, not WinMACCS. The developers intend to eliminate this restriction in the future so that partial or multiple years can be evaluated.

Transport dates

The transport dates are only required if there is weather sampling.

The variables on the ATMOS/HYSPLIT Transport/Transport Dates form are as follows:

HY_START is the first date for weather sampling. This is entered in MM/DD/YYYY format, for example "01/01/2008" is a valid string. Since the weather files used by HYSPLIT are in UTC time, this date is also defined for that time zone.

HY_END is the last date for weather sampling. This is entered in MM/DD/YYYY format, for example "12/31/2008" is a valid string. Since the weather files used by HYSPLIT are in UTC time, this date is also defined for that time zone.

Variable Name	Definable	Туре	Dimensions	Allowed Values
HY_START	Yes	String	None	10-character string of format MM/DD/YYYY
HY_END	Yes	String	None	10-character string of format MM/DD/YYYY

Extended time

The form *ATMOS/HYSPLIT Transport/Extended Time* allows for additional weather days before and after the starting and ending times for weather sampling. This form is required when the HYSPLIT model is selected for all weather options. The variables on this form are as follows: HY_BEFORE is the number of weather days preceding HY_START, the starting date for weather sampling. The purpose of these additional weather days is to allow for releases that are earlier than the MAXRIS plume segment that is aligned with the selected starting day and hour. For a fixed start time, this is the number of days preceding HY_FIXED that are supplied.

HY_AFTER is the number of weather days following HY_END when using weather sampling. Similarly, this is the number of days following HY_FIXED when using a fixed start time. The purpose for these additional days is to provide weather for plumes traveling through the grid after the end of the specified time interval, e.g., the end of a year of weather data. The user should choose a value of HY_AFTER sufficiently large so that the entire release can occur, and all plumes can transport through and out of the grid during the specified number of days.

Variable Name	Definable	Туре	Dimensions	Allowed Values
HY_BEFORE	Yes	Integer	None	0 to 2
HY_AFTER	Yes	Integer	None	0 to 40

Building height

The variable, HY_BUILDH, is the height of the building facility from which the release occurs. A value must be entered for every release. This value is used to evaluate whether a buoyant plume is entrained in the turbulent wake of the building.

Variable Name	Definable	Туре	Dimensions	Allowed Values
HY_BUILDH	Yes	Real	NUMREL	[1.0, 1000.0]

Specify model results

ATMOS results from the simulation are not specific to a plume segment when using the HYSPLIT model. Because of this, a different output request form is used to request Type 0 results. This form can be opened by double clicking on the form name *ATMOS/Output Control/Spatial Intervals* on the Parameters tab.

The ATMOS/Output Control/Spatial Intervals form is optional.

The variables on this form are as follows:

NUM0_HY specifies the number of Type 0 results to be created. For each request, seven results describing atmospheric transport and dispersion are reported. The value is automatically calculated by WinMACCS to be the number of rows in the grid containing values of INDRAD_HY.

INDRAD_ HY specifies the index of the radial grid element for which results are to be reported. The reported values are for the radial midpoint of the grid element.

When Report Options are set to CCDF or CCDF & REPORT, the complimentary cumulative distribution function data are reported in the MACCS output file. When set to REPORT or CCDF & REPORT, WinMACCS automatically generates a report over all realizations based on the quantile values specified on the *Reporting Options* form.

Variable Name	Definable	Туре	Dimensions	Allowed Values
NUM0_HY	Linked	Integer	None	0 to 35
INDRAD_HY	Yes	Integer	NUM_HY	1 to NUMRAD
Report Options	Yes	Character	NUM0	CCDF, NONE, REPORT, CCDF & REPORT

Running WinMACCS Using the MACCS-HYSPLIT Model

Clicking the Run Simulation starts a MACCS calculation. Before MACCS starts, the MACCS-HYSPLIT files are validated against the project settings. WinMACCS reports this process in the Results window. When the spatial grid, number of particle size bins, or the latitude and the longitude settings in WinMACCS are inconsistent with the MACCS-HYSPLIT data files, the MACCS run is not started and an error condition is reported to the user. WinMACCS also verifies that all the required files are available. The validation step stops if there is a discrepancy between what is expected in the files or if any files are missing. At the end of the validation step, WinMACCS reports the number of files processed provided that all files pass validation. The following shows the results window after a successful file validation.

Validating MACCS-HYSPLIT data files Completed validation of 1032 MACCS-HYSPLIT data files

The table below lists the set of tests done at this validation step.

WinMACCS	Validation	Remediation if validation does not
variable		pass
NUMCOR, number of sectors in grid	Equality with value in MACCS-HYSPLIT file header for each file	Rerun HyGridConvert
NUMRAD, number of radii in grid	Equality with value in MACCS-HYSPLIT file header for each file	Rerun HyGridConvert
SPAEND, radii used to define grid	For each value of SPAEND, and for each value of RADIUS in the MACCS-HYSPLIT file, validation passes if ABS(SPAEND – RADIUS) / ABS(SPAEND) <= 0.001	Rerun HyGridConvert
NPSGRP, number of particle size bins	Equality with value in MACCS-HYSPLIT file header	Rerun HYSPLIT with a consistent value for the number of particle size bins or modify number of particle size bins in WinMACCS to be consistent with HYSPLIT results
Latitude, site latitude	LAT is the latitude written to the MACCS-HYSPLIT file and Latitude is the value in WinMACCS, validation passes if ABS(Latitude – LAT) <= 0.01, which corresponds to approximately 1 km at the equator	Rerun HYSPLIT. Location of data site being modeled is not consistent with HYSPLIT results
Longitude, site longitude	If LONG is the longitude written to the MACCS-HYSPLIT file, validation passes if ABS(Longitude - LONG) <= 0.01, which corresponds to approximately 1 km	Rerun HYSPLIT. Location of data site being modeled is not consistent with HYSPLIT results

When weather files are missing, then the MACCS run is not started. In this case, HYSPLIT may need to be run to create the missing files, following by running HyGridConvert to convert the HYSPLIT output into MACCS-HYSPLIT files.

The required files are shown in the following table:

Sampling Method	Files Required	Example
Fixed Start Time	24 files associated with a weather	HY_FIXED = "06/01/2008"
(METCOD = 1)	day defined in WinMACCS	HY_BEFORE = 1
	variable HY_FIXED, plus files	$HY_AFTER = 2$
	associated with HY_BEFORE	If there is exactly one value of
	days before HY_FIXED and	HY_PREFIX, and
	HY_AFTER days following	HY_PREFIX[1]="H001" then there
	HY_FIXED. A complete set of	are 24 files/day *4 days, or 96 files
	files is expected for each value of	required, starting with
	variable HY_PREFIX.	2008053100H001.mcd and ending
		with 2008060323HY001.mcd
Weather	24 files per day for all days in the	HY_START = "01/01/2008"
Sampling	interval defined by WinMACCS	HY_END = "12/31/2008"
	variables HY_START and	HY_BEFORE = 2
	HY_END, plus files associated	$HY_AFTER = 15$
	with HY_BEFORE days before	If there is exactly one value of
	HY_START and HY_AFTER	HY_PREFIX, and
	days following HY_END	HY_PREFIX[1]="P050" then there
		are 24 files/day * (2 days + 366 days
		+ 15 days), or 9192 files required,
		starting with 2007123000P050.mcd to
		2009011523P050.mcd

MACCS-HYSPLIT Model Results

Basic air and ground concentration results are available when using the HYSPLIT atmospheric transport option. These are analogous to the results that can be obtained for the Gaussian plume segment option, but not identical. For example, the concept of a plume centerline does not exist in the HYSPLIT model, so centerline is replaced by peak, which has the meaning of the maximum value around the compass at a distance corresponding a circle at the center of a ring. The table below provides a description of the Type 0 outputs that are created when using the HYSPLIT transport model.

Result	Description
Peak Ground-Level Air Concentration (Bq·s/m³)	Peak (around the compass), time-integrated, ground-level, air concentration for the selected radionuclide at the requested distance
Peak Ground Concentration (Bq/m²)	Peak (around the compass) ground concentration for the selected radionuclide at radionuclide exit time at the requested distance
Total Peak Ground Concentration (Bq/m²)	Peak (around the compass) ground concentration for all radionuclides at radionuclide exit time at the requested distance
Adjusted Source Strength (Bq)	Inventory of the selected radionuclide at radionuclide exit time accounting for decay and deposition
Ground-Level Chi/Q (s/m ³)	Peak (around the compass) time-integrated, ground-level, air concentration for the selected radionuclide divided by the adjusted source at the same distance
Radionuclide Arrival Time (s)	First time at which a non-zero ground-level air concentration of the selected radionuclide crosses the midpoint of a ring
Radionuclide Exit Time (s)	Last time at which a non-zero ground-level air concentration of the selected radionuclide crosses the midpoint of a ring

WinMACCS Sample Problem - HYSPLIT Fixed Start Time

Locate HYSPLIT Data

To generate HYSPLIT files for use with this project, follow the steps in the section, HYSPLIT Sample Problem, Five Days of Data, above to create the five days of HYSPLIT files before running the problem in WinMACCS.

Sample output files from the GenHysplit program (the program that runs HYSPLIT to create atmospheric transport results) are provided in the distribution folder \Sample Problems\ HYSPLIT_files_fixed_start. These files have an extension ".ccd". It is not necessary to run GenHysplit (and hence HYSPLIT) if the provided files are used.

Sample output files from HyGridConvert utility (the program that converts the output from GenHysplit to the MACCS input format) are provided in the distribution folder \Sample Problems\MACCS_files_fixed_start. These files have an extension ".mcd". It is not necessary to run GenHysplit (and hence HYSPLIT) or HyGridConvert if the provided files are used.

Create Project

Start WinMACCS.

Select *File/Open Project* from the main menu. Open the project file *Gaussian Fixed Start Time.mxd*.

Select *File/SaveAs* Project from the main menu. Enter *HYSPLIT Fixed Start Time* in the *Project Name* text box. Click *OK*.

Select the HYSPLIT Model

Select *Edit/Project Properties* from the main menu. In the *Project Properties* form on the *Scope* tab change the *Atmospheric Transport and Dispersion* option from *Gaussian* to *HYSPLIT*. Click on the *Weather* tab. Notice that *Fixed Start Time* is selected. Click *OK* to save.

Define the MACCS-HYSPLIT Variables

Using HyGridConvert, a utility that WinMACCS uses to generate the .mcd files from .ccd files, a set of input files (.mcd) have already been created for use in this sample problem. The basic difference between these files is that .ccd files contain air and ground concentrations for the grid defined in the HYSPLIT calculation. The .mcd files contain air and ground concentrations interpolated onto the MACCS grid. These .mcd files can either be used directly for the sample problem or as comparison files after following the process below.

If it is necessary or desired to create .mcd files from the .ccd files, do the following:

Select PreProcessing/Create MACCS-HYSPLIT files from the main menu.

Click the *Browse* ... button next to *HYSPLIT File Folder* text box and select folder containing GenHysplit output (.ccd) files.

Click the *Browse* ... button next to *Folder for Results* text box and select folder where you wish to store the desired MACCS input files (.mcd).

Click the *Convert* button. This will begin the conversion process and may take 1-2 minutes.

After the conversion is complete, answer *Yes* to have this folder automatically linked to this project. If this is done, there is no need to manually link this folder using the form *GENERAL/FileSpecifications/HYSPLIT Converted Folder*.

Specify the location of the MACCS-HYSPLIT files

This may not be necessary if the folder was linked from the form *PreProcessing/Create MACCS-HYSPLIT files*. Sample .mcd files have been included in the distribution folder \Sample Problems\MACCS_files_fixed_start. To use the provided files, click on the plus sign next to the *GENERAL/File Specifications* entry. Double click on the form name *HYSPLIT Converted Folder*. Click the *Browse* ... button next *to MACCS-HYSPLIT files* text box and select the folder containing the set of MACCS input files (.mcd) to be used in this calculation.

Click OK.

Indicate the MACCS-HYSPLIT weather files and when to use them Open the form ATMOS/HYSPLIT Transport/File Extensions and Lower Bounds.

Fill in the grid as shown in Figure 3 and then click *OK*.

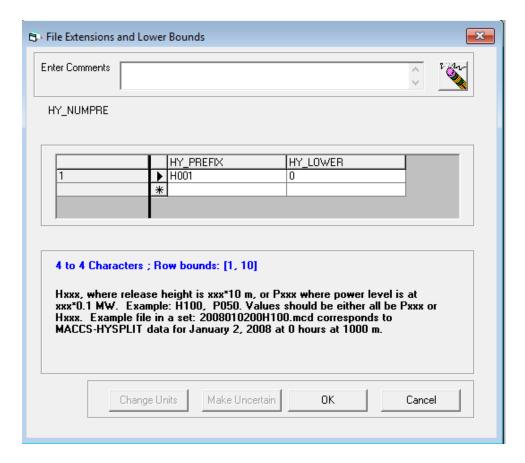


Figure 3. Define File Names and Lower Bounds

This specifies that all releases above ground level (0 m) are to be treated using a file(s) ending in H001. Multiple release heights can be represented by specifying multiple files sets with different endings.

Define time intervals

Open the form ATMOS/HYSPLIT Transport/Fixed Start Time Data.

Fill in the grid as is shown in Figure 4 and then click *OK*.

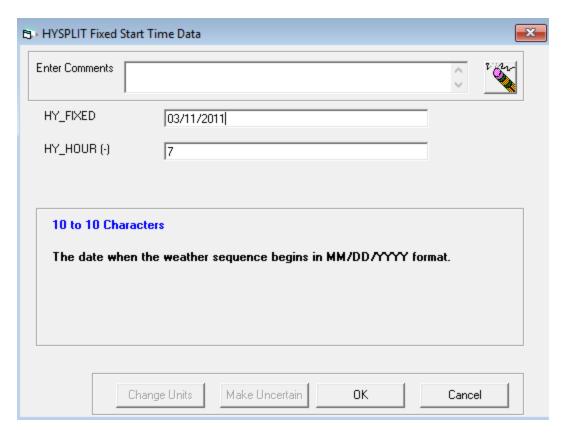


Figure 4. Enter Start Time

Open the form ATMOS/HYSPLIT Transport/Extended Time.

Fill in the form as is shown in Figure 5 and then click OK.

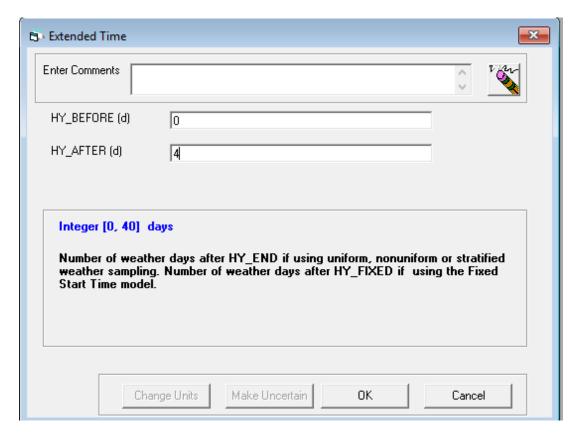


Figure 5. Extended Time

These choices indicate that no weather is specified prior to the starting day and 4 days are specified following the starting day. This allows releases to occur for a maximum of 5 consecutive days.

Define building height for each plume release

Open the form ATMOS/HYSPLIT Transport/HYSPLIT Building Height.

Fill in the form as is shown in Figure 6 and then click *OK*.

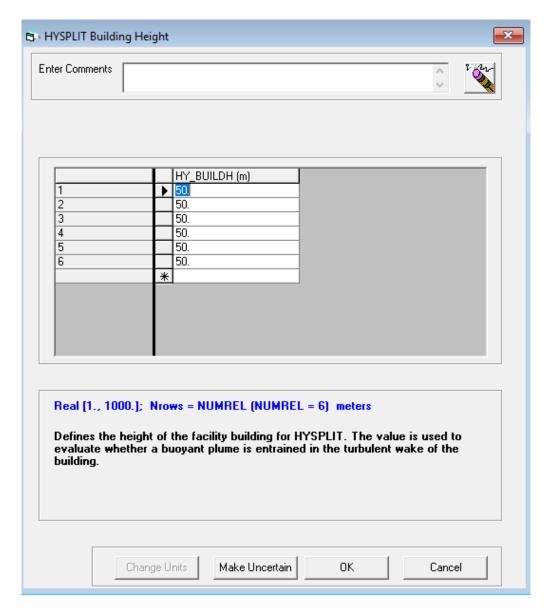


Figure 6. Building Height for Each Plume

Run the MACCS-HYSPLIT Model

Select Execute/Run Models from the main menu. Click the Run Simulation button.

This generates a Model1.bin and Model1.out file in the Output folder. Comparison of the Model1.out file can be made with the "HYSPLIT Fixed Start Time.out" file included in the Output folder of the project *Gaussian Fixed Start Time*.

The output files from GenHysplit used in this calculation were created using a Linux operating system running HYSPLIT version 945. There may be minor differences in the results when the version of HYSPLIT is different or HYSPLIT was run under a different operating system.

WinMACCS Sample Problem - HYSPLIT Weather Sampling

Locate HYSPLIT Data

To generate HYSPLIT files for use with this project, follow the steps in section HYSPLIT Sample Problem, One Year of Data above to create the one year of HYSPLIT files before running the problem in WinMACCS. WinMACCS can then be used to convert the ".ccd" files using the HyGridConvert utility as discussed in section WinMACCS Sample Problem – HYSPLIT Fixed Start Time above.

Sample output files from the GenHysplit program (the program that runs HYSPLIT to create atmospheric transport results) and processed through the HyGridConvert utility (the program that converts the output from GenHysplit to the MACCS input format) are provided in the distribution folder \Sample Problems\MACCS_files_weather_sampling. These files have an extension ".mcd". It is not necessary to run GenHysplit (and hence HYSPLIT) or HyGridConvert if the provided files are used.

Create Project

Start WinMACCS.

Select *File/Open Project* from the main menu. Open the project file *Gaussian Weather Sampling.mxd*.

Select *File/SaveAs* Project from the main menu. Enter *HYSPLIT Weather Sampling* in the *Project Name* text box. Click *OK*.

Select the HYSPLIT Model

Select Edit/Project Properties from the main menu. In the Project Properties form on the Scope tab change the Atmospheric Transport and Dispersion option from Gaussian to HYSPLIT. Click on the Weather tab. Notice that Nonuniform Bin Sampling is selected. Click OK to save.

Define the MACCS-HYSPLIT Variables

Specify the location of the MACCS-HYSPLIT files

On the *Parameters* tab of the *Project* window, click on the plus sign next to the *GENERAL/File Specifications* entry. Double click on the form name *HYSPLIT Converted Folder*. Click on text box next to the words *MACCS-HYSPLIT files*. Note that a comment appears in the area below this text box describing the required input. To satisfy this input requirement, click the *Browse* ... button next *to MACCS-HYSPLIT files* text box and select the folder containing the set of MACCS input files (files with the extension .mcd) to be used in this calculation. Click *OK*.

A set of input files (.mcd) have already been created using GenHysplit (which runs HYSPLIT), and a utility that can be run from WinMACCS called HyGridConvert. When the spatial grid definition is changed (WinMACCS variables SPAEND or NUMCOR), HyGridConvert needs to

recreate the .mcd files. If the site location (Latitude or Longitude), the number of aerosol size bins, or the aerosol sizes change, HYSPLIT must be rerun.

The sample .mcd files can be found in the distribution folder \Sample Problems\MACCS_files_weather_sampling

Indicate the MACCS-HYSPLIT concentration files and when to use them Open the form ATMOS/HYSPLIT Transport/File Extensions and Lower Bounds.

Not all files in the *MACCS-HYSPLIT files* folder are used in a calculation. The release height and the power used in the GenHysplit calculation are encoded in the file name. The calculation can be based on either height (using H in the HY_PREFIX variable) or power (using P in the HY_PREFIX variable), but not a mixture of both.

The variable HY_LOWER determines when the associated files are used. Notice, the units of HY_LOWER are in meters in this example because only files with an H is the postfix portion of their names (H001, H005 and H010) are used. H001 (representing a release height of 10 m) is used for release heights in the range of 0 to less than 30 m. H005 (representing a release height of 50 m) is used for release heights from 30 to less than 75 m. H010 (representing a release height of 100 m) is used for heights greater than or equal to 75 m.

Fill in the grid as is shown in Figure 7 and then click *OK*.

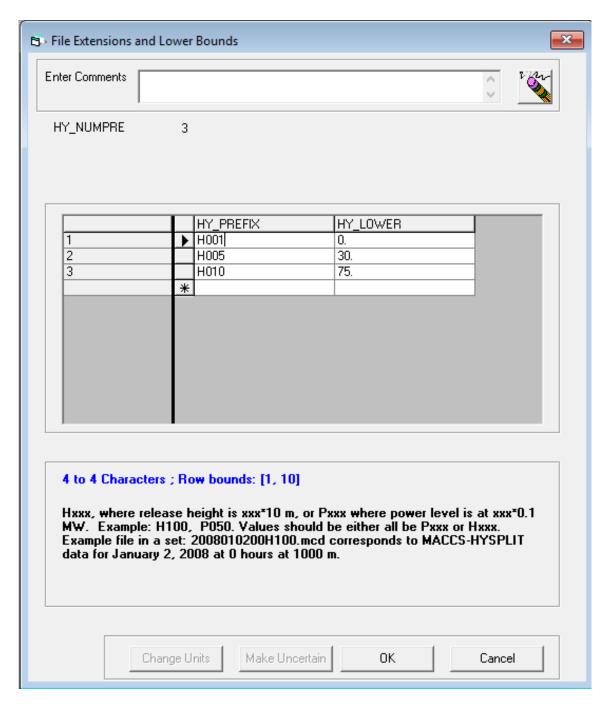


Figure 7. Form to Define File Names and Lower Bounds

Indicate the dates to use in the model

Open the form ATMOS/HYSPLIT Transport/Transport Dates.

The software expects 24 files for each one of these days to be present in the *MACCS-HYSPLIT* files folder for each of the height or power specified on the File Extensions and Lower Bounds form.

Fill in the form as is shown in Figure 8 and then click *OK*.

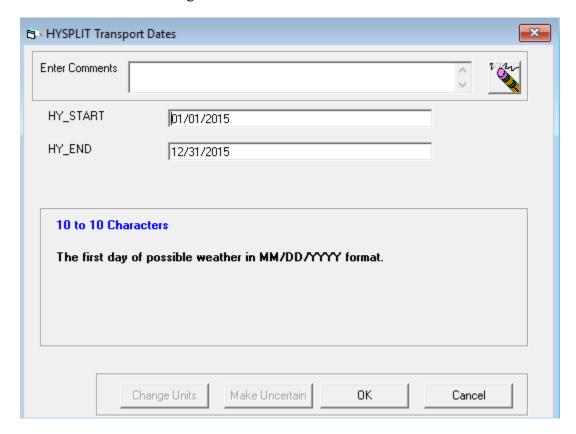


Figure 8. Define Time Interval

Open the form ATMOS/HYSPLIT Transport/Extended Time.

The software expects 24 files for each date from HY_BEFORE to HY_START and HY_END to HY_AFTER.

Fill in the form as is shown in Figure 9 and then click *OK*.

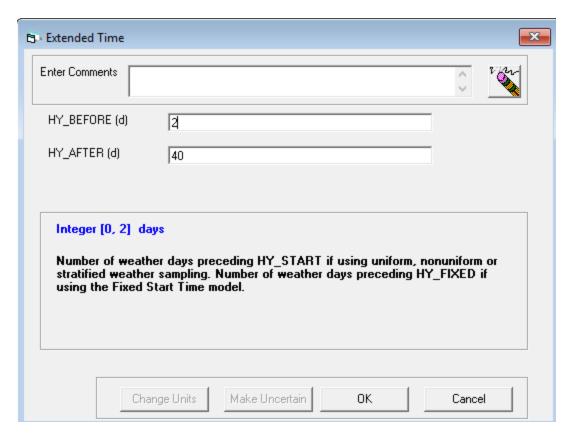


Figure 9. Define Extended Time Intervals

Under "ATMOS", "HYSPLIT Transport", click on "Building Height". Enter 50 for both rows of HY_BUILD. Click "OK".

Define building height for each plume release

Open the form ATMOS/HYSPLIT Transport/HYSPLIT Building Height.

Fill in the form as is shown in Figure 10 and then click *OK*.

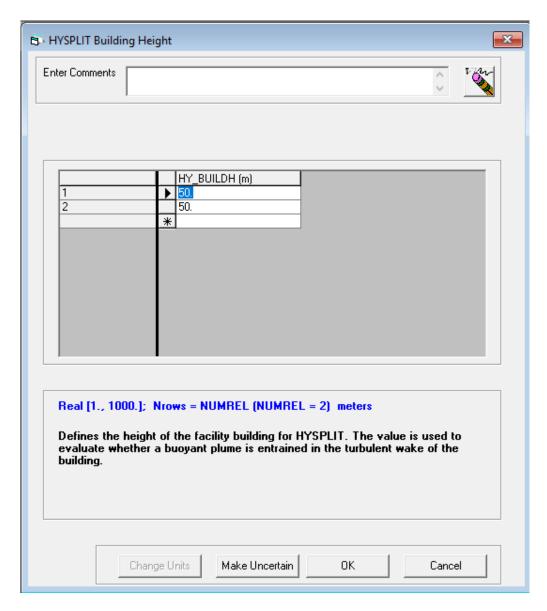


Figure 10. Form to Define Building Height for Each Plume Segment

Run the MACCS-HYSPLIT Model

Select Execute/Run Models from the main menu. Click the Run Simulation button.

This should generate a Model1.bin and Model1.out file in the Output folder. Comparison of the Model1.out file can be made with the "HYSPLIT Weather Sampling.out" file included in the Output folder of the project *Gaussian Weather Sampling*.

The output files from GenHysplit used in this calculation were created using a Linux operating system running HYSPLIT version 945. There may be minor differences in the results when either the version of HYSPLIT is different or HYSPLIT was run on a different operating system.